

# Procedure for Eliminating Aromatic Bond Representations from SDF Files using CambridgeSoft ChemFinder (ver. 7.0) and ACD ChemFolder (ver 6.0)

(27 June 03)

*In many cases, we have Main ChemFinder files that contain aromatic bonds represented in special form in the structure view, i.e. as circle inside ring. Upon export to SDF, ChemFinder uses a special number code for these bonds that is not universally recognized in other Chemical Relational Database applications. Upon import of the SDF file into ACD ChemFolder, and reexport of this file, the special aromatic bond designation is eliminated, but ChemFolder adds extraneous fields that must be deleted using ChemFinder. To convert structures to explicit bond representation (i.e., alternating single and double bonds in aromatic ring) and eliminate extraneous fields in the SDF, we use the following procedure.*

1. Open SDF file in ChemFinder.
2. Select **Export -> SDF file** from the **File** menu, and save to SDF file name in new sub folder titled "Final SDF generated from ACD ChemFolder".
3. Launch ChemFinder and import SDF file just produced from ACD ChemFolder.
4. Check to see that aromatic rings no longer represented with circle in ring.
5. Save and close ChemFinder. Launch corresponding \*.mdb file in MS Access.
6. Click on Field Design button in top menu bar (blue triangle).
7. Delete fields "FW" and "ID" generated from ACD ChemFolder export.
8. Close file and MS Access. Launch ChemFinder and check to see that fields have been deleted. Click arrow button on left menu bar, select and delete boxes corresponding to FW and ID fields.
9. **File -> Export -> SDF file**, rewriting over previous SDF file.
10. Copy and paste this revised SDF file over the previous SDF file in Main folder.